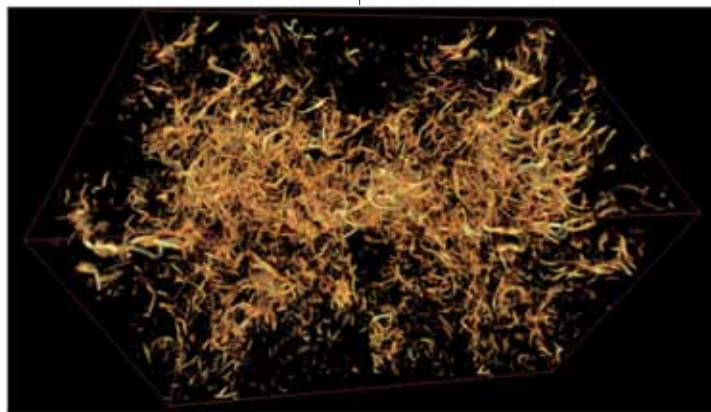


Direct Numerical Simulations of Reacting Compressible Turbulence

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Fig. 1. Enstrophy field in reacting compressible turbulence shows the rich phenomenology of the flame turbulence interaction. The very high resolution simulations highlight the presence of vortex tubes. Across the flame, fire polishing damps the smallest turbulence scales; however some of the vortex tubes are enhanced through baroclinic vorticity generation.



Although important progress has been made in recent years in our understanding of turbulence, complete quantification, description, prediction, simulation, and control still elude us. The problem is due in part to the very large range of spatio-temporal, dynamically relevant scales, but also to the multitude of problems that can be encompassed by the generic term turbulence. If ideal turbulence is in a homogeneous, isotropic Kolmogorov steady state, then nonideal turbulence can occur due to most practically relevant effects: time-dependence, anisotropy, inhomogeneity, coupling with active scalars, shock waves, exothermic reactions, etc. Unlike kinetic theory, where significant departure from a weakly perturbed local Maxwellian is exceptional, the analogous state of nonideal turbulence is what is typical, yet the only successful turbulence theory so far is Kolmogorov's 1941 theory. It is then not surprising that the turbulence theory is still centered on the ideas of Kolmogorov related to the existence of inertial range dynamics (e.g., a $-5/3$ range in the isotropic turbulence energy spectrum) and small scale universality. However, more and more evidence points to departures from universal laws in the energy spectrum due to intermittency and a

direct connection between the small and the (nonuniversal) large scales, especially in the presence of strong gradients [1] or buoyancy [2-4].

Most of the turbulence research to date has been concentrated on several canonical flows with periodic boundaries or simple jets, wakes, or boundary layers. Numerous modeling strategies have been proposed, and, while

there is no best strategy, each of the approaches has its own advantages and domains of applicability. Yet most practical flows are not canonical. In many situations, they are driven by acceleration as in ICF or cosmic explosions and may undergo exothermic reactions. In addition, radiation could have a significant effect, e.g., through heat gain or loss. For these complex flows, the limitations of the current modeling strategies, as well as the turbulence and mixing properties are unknown.

Turbulence theory and the subsequent model development rely on experimental or high resolution direct numerical simulations (DNS) data for development and verification and validation. This technique has emerged as a powerful research tool to study the physics of turbulence, verify and improve models, complement and even guide and help design better experiments [5]. The DNS technique seeks exact solutions of the governing equations, so that all relevant scales are accurately solved, using high resolution numerical simulations based on high-order accurate discretization algorithms. DNS rely on nondissipative high accuracy schemes and are conducted without resort to subgrid modeling or the introduction of artificial numerical dissipation or other algorithm stabilizing schemes. Such computations allow a degree of control in isolating specific physical phenomena that is typically inaccessible in experiments. With the recent advances in supercomputing technology and algorithms, it is now possible to perform simulations of simple flows at ranges of scales comparable to or even larger than in typical laboratory experiments. Petascale computing is expected to further increase the range of scales of the simulations and allow accurate calculations of more and more complex flows.

This study represents the first successful implementation of a large structured fluid dynamics code (CFDNS) on the IBM Cell Broadband Engine (Cell BE) architecture. The CFDNS code solves the compressible and incompressible Navier-Stokes equations in 3D using high-order compact finite differences or Fourier transforms in the periodic directions. Multiple species are allowed, each with realistic material properties and equations of state (EOS), as well as Cartesian, cylindrical, and spherical grid geometries. The serial speedup of the Cell BE version of the code is approximately 30x, which is

reasonable when considering the clock speed, parallelism and vectorization afforded by the Cell BE. Notably, the excellent performance of the individual memory controllers is responsible for this, since the low arithmetic intensity of the algorithm does not allow the actual compute power of the Cell's synergistic processing elements (SPEs) to be utilized. This serial speedup prompted us to perform significant modifications to the parallel code design, as indicated above, which lead to overall speedup in the range of 20x compared with the AMD Opteron-only version [6,7].

The model problem addressed by the study is the flame-turbulence interaction under the complex conditions characterizing the early stages of a type Ia supernova. These conditions are novel and have no direct analogue on earth. This makes them interesting for testing new physics, but it also means that our terrestrial intuition regarding flames can be misleading. For example, it is thought that laboratory flames in the $Ka \gg 1$ regime simply go out because they are unable to maintain their heat in the presence of so much turbulence. But the flame in a supernova can never go out until the star comes apart and, in terms of local flame variables, that takes a very long time. Although several mechanisms for detonation have been proposed, the debate around deflagration/detonation models is still not settled. Moreover, most turbulent flame simulations so far, under these conditions, are in the low Mach number approximation and no DNS have been performed for such flows.

Using the Roadrunner supercomputer, researchers have performed the largest reacting compressible turbulence simulations to date. The flow conditions considered for the reacting simulations correspond to well-stirred single component burning, $^{12}\text{C}(^{12}\text{C},\text{g})^{24}\text{Mg}$, relevant to Type Ia supernovae. The flame advances into the cold fuel (^{12}C) in a C-O mixture and leaves behind hot product (^{24}Mg). Inflow/outflow boundary conditions are imposed in the flame propagation direction. The physical transport properties are appropriate for the astrophysical situation investigated and are calculated within new modules added to the code. Thus, the thermal transport includes both radiative and electron transport (accounting for degenerate regimes) contributions. The equation of state considers radiative, ion, and electron contributions. To reduce the computational effort, precomputed tables for the

transport properties, EOS, and nuclear energy rates are used.

The simulations were performed in stages: a) generate 1D reacting flow profiles as initial conditions, b) generate inflow turbulence by performing triply periodic simulations with a background velocity matching the flame speed [8], and c) flame-turbulence interaction under supernova conditions. To better study the flame characteristics, the reference frame was chosen such that the flame was stationary in the computational domain. The 3D reacting flow simulations were initialized using the 1D profiles and isotropic turbulence was introduced through the inflow boundary. To understand the effects of various parameters, most notably Da and Ka numbers, as well as the effect of compressibility, several simulations were performed on up to 2048^3 meshes.

There is a complicated phenomenology associated with turbulent flames under type Ia supernova conditions from the suppression of the smallest vortex tubes due to the flame fire polishing, but enhancement of intermediate turbulent scales (Fig. 1), to the rapid acceleration of the flame itself to large velocities, is one of the important open questions related to the supernova modeling. In addition, the fully compressible simulations allowed considering the dynamics of the dilatational motions, neglected in previous studies. These motions are enhanced by the heat addition due to the flame and can cause shock waves that may lead to detona-

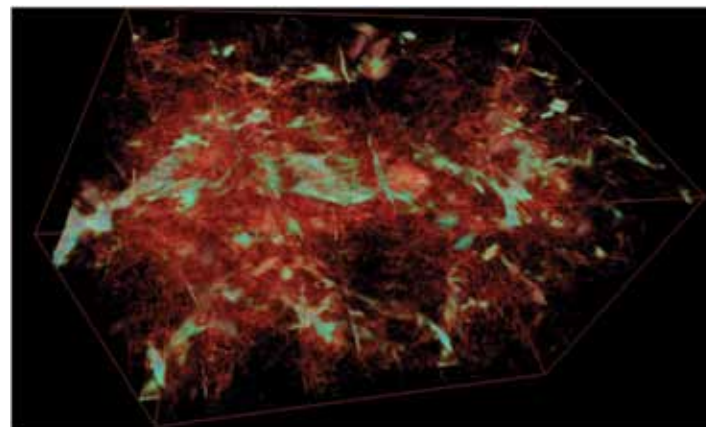


Fig. 2. Dilatational effects, usually neglected in astrophysical calculations, are important for understanding the deflagration-detonation initiation. Our results indicate the presence of shocklets, generated by the turbulence and enhanced by the dilatational motions due to the flame. Sufficiently strong shocklets may be the mechanism for producing detonation in type Ia supernovae.

tion (Fig. 2). Current research focuses on the departures of the turbulence properties from the classical Kolmogorov picture and determining accurate turbulent flame speeds.

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Funding Acknowledgments

LANL Directed Research and Development Program—Exploratory Research (ER)